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Reply to the comment on spontaneous magnetization of simple metal nanowires

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Zabala, Puska, and Nieminen Reply: The Lieb-Mattis (LM) theorem [1] proves that for interacting fermions in strictly one dimension, the ground state of the system has the lowest possible spin. The requirement for the interaction is that it not be “pathological.” An example of a pathological potential is an infinite repulsive core.

The essential ingredient in the LM theorem is that it is possible to specify a quantum state in terms of one simplex in configuration space. The one-dimensional character is that the action of the Hamiltonian can be described in terms solely of one simplex $x_1 < x_2 < x_3 < \dots$. In terms of a tight-binding model, this means that there is no hopping from one simplex to another without passing through the boundary.

The LM theorem does not apply for the case of cylindrical wire considered in Ref. [2]. The wire is three dimensional, with a finite transverse width. For this geometry, even with just a single subband occupied, the interaction potential should be separately symmetric in all three coordinates. The Coulomb potential between electrons does not satisfy the requirement, as was, in fact, stated explicitly in the original paper [1]. We thus conclude that the LM theorem cannot be used to rule out ferromagnetism in quantum wires, contrary to what is asserted by Starykh and Maslov [3].

Another question is how reliable a mean-field-type, spin-density-functional formulation is in predicting magnetic structures in confined geometries. For example, the spin-density-functional theory, where S_z only is a good spin quantum number, can lead to spurious symmetry breaking. A two-dimensional quantum dot with degenerate angular momentum states is a case in point [4]. For

the 3D wire, a spin-Peierls state along the wire direction is another possible outcome of the spin-density-functional theory. However, in our Letter we make no quantitative predictions of such states.

The system discussed in Ref. [2] is actually better viewed as a model of thin metal wires where there is a gradual confinement of quantum states perpendicular to the wire direction. The ultimate limit is the atomic chain. We have also performed local-spin-density calculations for such chains. For example, a chain of Al atoms with an interatomic distance corresponding to that in bulk Al exhibits a spin-polarized p_{xy} -type subband in good agreement with the stabilized jellium prediction [2].

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